

STN Columbus

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page for STN Seminar Schedule - N. America
NEWS 2 OCT 02 CA/CAPLUS enhanced with pre-1907 records from Chemisches
Zentralblatt
NEWS 3 OCT 19 BEILSTEIN updated with new compounds
NEWS 4 NOV 15 Derwent Indian patent publication number format enhanced
NEWS 5 NOV 19 WPIX enhanced with XML display format
NEWS 6 NOV 30 ICSD reloaded with enhancements
NEWS 7 DEC 04 LINPADOCDB now available on STN
NEWS 8 DEC 14 BEILSTEIN pricing structure to change
NEWS 9 DEC 17 USPATOLD added to additional database clusters
NEWS 10 DEC 17 IMSDRUGCONF removed from database clusters and STN
NEWS 11 DEC 17 DGENE now includes more than 10 million sequences
NEWS 12 DEC 17 TOXCENTER enhanced with 2008 MeSH vocabulary in
MEDLINE segment
NEWS 13 DEC 17 MEDLINE and LMEMLINE updated with 2008 MeSH vocabulary
NEWS 14 DEC 17 CA/CAPLUS enhanced with new custom IPC display formats
NEWS 15 DEC 17 STN Viewer enhanced with full-text patent content
from USPATOLD
NEWS 16 JAN 02 STN pricing information for 2008 now available
NEWS 17 JAN 16 CAS patent coverage enhanced to include exemplified
prophetic substances
NEWS 18 JAN 28 USPATFULL, USPAT2, and USPATOLD enhanced with new
custom IPC display formats
NEWS 19 JAN 28 MARPAT searching enhanced
NEWS 20 JAN 28 USGENE now provides USPTO sequence data within 3 days
of publication
NEWS 21 JAN 28 TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 22 JAN 28 MEDLINE and LMEMLINE reloaded with enhancements
NEWS 23 FEB 08 STN Express, Version 8.3, now available
NEWS 24 FEB 20 PCI now available as a replacement to DPCI
NEWS 25 FEB 25 IFIREF reloaded with enhancements
NEWS 26 FEB 25 IMSPRODUCT reloaded with enhancements
NEWS 27 FEB 29 WPINDEX/WPIDS/WPIX enhanced with ECLA and current
U.S. National Patent Classification

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 22:16:47 ON 26 MAR 2008

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 22:16:58 ON 26 MAR 2008
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 25 MAR 2008 HIGHEST RN 1010115-69-1
DICTIONARY FILE UPDATES: 25 MAR 2008 HIGHEST RN 1010115-69-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=> e rapamycin/cn

E1	1	RAPAMMUNE/CN
E2	1	RAPAMUNE/CN
E3	1 -->	RAPAMYCIN/CN
E4	1	RAPAMYCIN 29-ENOL/CN
E5	1	RAPAMYCIN 31-O-METHYLTRANSFERASE/CN
E6	1	RAPAMYCIN 42-(BENZYL SUCCINATE)/CN
E7	1	RAPAMYCIN 42-(METHYL SUCCINATE)/CN
E8	1	RAPAMYCIN 42-HEMIADIPATE/CN
E9	1	RAPAMYCIN 42-HEMISUCCINATE/CN
E10	1	RAPAMYCIN ASSOCIATED PROTEIN (CARASSIUS AURATUS FRAGMENT)/CN
E11	1	RAPAMYCIN ASSOCIATED PROTEIN FRAP2 (HUMAN CLONE 99P18 GENE F RAP2 C-TERMINAL FRAGMENT)/CN
E12	1	RAPAMYCIN DIACETATE/CN

=> s e3

L1 1 RAPAMYCIN/CN

=> d

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN

RN 53123-88-9 REGISTRY

ED Entered STN: 16 Nov 1984

CN **Rapamycin** (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 23,27-Epoxy-3H-pyrido[2,1-c][1,4]oxaazacyclohentriacontine, rapamycin deriv.

OTHER NAMES:

CN (-)-Rapamycin

CN (3S,6R,7E,9R,10R,12R,14S,15E,17E,19E,21S,23S,26R,27R,34aS)-9,10,12,13,14,21,22,23,24,25,26,27,32,33,34,34a-Hexadecahydro-9,27-dihydroxy-3-[(1R)-2-[(1S,3R,4R)-4-hydroxy-3-methoxycyclohexyl]-1-methylethyl]-10,21-dimethoxy-6,8,12,14,20,26-hexamethyl-23,27-epoxy-3H-pyrido[2,1-c][1,4]oxaazacyclohentriacontine-1,5,11,28,29(4H,6H,31H)-pentone

CN 23,27-Epoxy-3H-pyrido[2,1-c][1,4]oxaazacyclohentriacontine-1,5,11,28,29(4H,6H,31H)-pentone, 9,10,12,13,14,21,22,23,24,25,26,27,32,33,34,34a-hexadecahydro-9,27-dihydroxy-3-[2-(4-hydroxy-3-methoxycyclohexyl)-1-methylethyl]-10,21-dimethoxy-6,8,12,14,20,26-hexamethyl-, [3S-[3R*[S*(1R*,3S*,4S*)],6S*,7E,9S*,10S*,12S*,14R*,15E,17E,19E,21R*,23R*,26S*,27S*,34aR*]]-

CN Antibiotic AY 22989

CN AY 22989

CN NSC 226080

CN RAPA

CN Rapammune

CN Rapamune

CN RPM

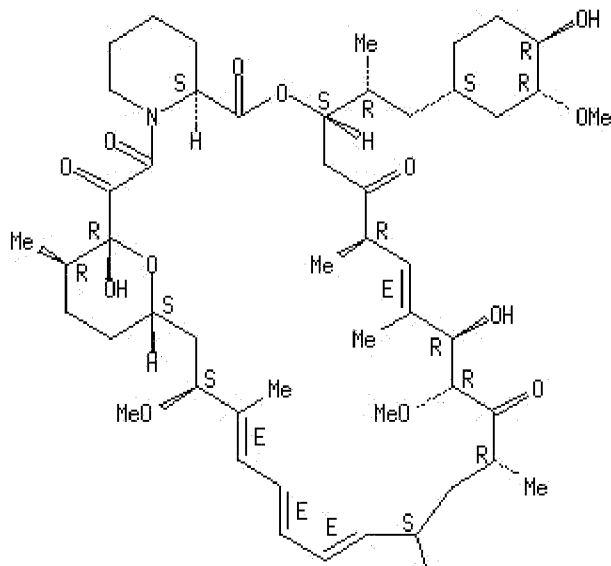
CN SIIA 9268A

CN Sirolimus

CN Wy 090217
 CN [3S-[3R*[S*(1R*,3S*,4S*)],6S*,7E,9S*,10S*,12S*,14R*,15E,17E,19E,21R*,23R*,
 26S*,27S*,34aR*]]-9,10,12,13,14,21,22,23,24,25,26,27,32,33,34,34a-
 Hexadecahydro-9,27-dihydroxy-3-[2-(4-hydroxy-3-methoxycyclohexyl)-1-
 methylethyl]-10,21-dimethoxy-6,8,12,14,20,26-hexamethyl-23,27-epoxy-3H-
 pyrido[2,1-c][1,4]oxaazacyclohentriacontine-1,5,11,28,29(4H,6H,31H)-
 pentone
 FS STEREOSEARCH
 MF C51 H79 N O13
 CI COM
 LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS,
 BIOTECHNO, CA, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN,
 CSCHEM, DDFU, DRUGU, EMBASE, HSDB*, IFICDB, IFIPAT, IFIUDB, IMSDRUGNEWS,
 IMSPATENTS, IMSPRODUCT, IMSRESEARCH, IPA, MEDLINE, MRCK*, MSDS-OHS,
 NAPRALERT, PATDPASPC, PHAR, PROMT, PROUSDDR, PS, RTECS*, SYNTHLINE,
 TOXCENTER, USAN, USPAT2, USPATFULL, VETU
 (*File contains numerically searchable property data)
 Other Sources: WHO

Absolute stereochemistry.
 Double bond geometry as shown.

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PAGE 2-A



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5162 REFERENCES IN FILE CA (1907 TO DATE)
 325 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 5194 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file merck
 COST IN U.S. DOLLARS
 FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
7.61	7.82

FILE 'MRCK' ENTERED AT 22:17:20 ON 26 MAR 2008
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=> s l1

L2 1 L1

=> d all

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MERCK Number (MNO): 8202

CAS Registry No. (RN): **53123-88-9**

MERCK Index Name (MIN): Rapamycin

Synonym(s) (CN): Sirolimus; RAPA; RPM

Drug Code(s) (CN): AY-22989; NSC-226080

Trade Name(s) (CN): Rapamune (Wyeth)

Molecular Form. (MF): C₅₁ H₇₉ N O₁₃

Wgt Composition (COMP): C 67.01%, H 8.71%, N 1.53%, O 22.75%.

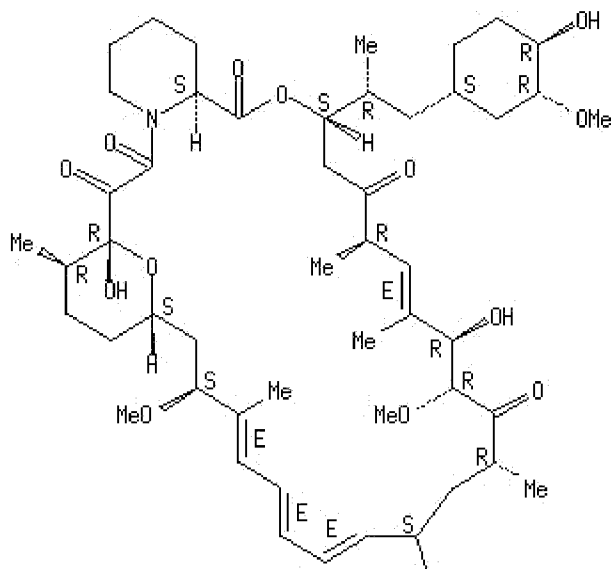
Molecular Weight (MW): 914.17

References (RE): Triene macrolide antibiotic isolated from *Streptomyces hygroscopicus*. Name derived from the native word for Easter Island, Rapa Nui. Isoln: S. N. Sehgal et al., DE 2347682; eidem, US 3929992 (1974, 1975 both to Ayerst McKenna Harrison); purification and characterization: C. Vezina et al., J. Antibiot. 28, 721 (1975); S. N. Sehgal et al., ibid. 727. Inhibition of immune response: R. R. Martel et al., Can. J. Physiol. Pharmacol. 55, 48 (1977); of graft rejection in mice: C. P. Eng et al., Transplant. Proc. 23, 868 (1991). Total synthesis: K. C. Nicolaou et al., J. Am. Chem. Soc. 115, 4419 (1993); D. Romo et al., ibid. 7906. Series of articles on therapeutic monitoring and pharmacokinetics: Clin. Ther. 22, Suppl. 2, B1-B132 (2000); on pharmacology and clinical experience in transplantation: Transplant. Proc. 35, Suppl. 1, S1-S233 (2003). Clinical trial in prevention of coronary restenosis: D. R. Holmes, Jr. et al., Circulation 109, 634 (2004).

Absolute stereochemistry.

Double bond geometry as shown.

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PAGE 2-A

Me

Melting Point (MP):

Value
MP
deg C
=====

183 - 185

Optical Rotatory Power (ORP):

Value	Temp.	Spectral Line	Note
ORP	ORP.T	ORP.SL	
deg	deg C		
-58.2	25	D	(methanol)

Toxicity (TOX):

LD50 in mice (mg/kg): 600 i.p.; >2,500 orally (Vezina).

UV Spectrum (UVS):

Maximum Peak Pos.	Note
UVS.PP nm	
267	(95% ethanol) (E1%1cm 417, 541, 416)
277	
288	

Other Properties (OCP):

Colorless crystalline solid from ether, mp 183-185° . uv max (95% ethanol): 267 , 277 , 288 nm (E1%1cm 417, 541, 416) . [α]D25 -58.2° (methanol) . Sol in ether, chloroform, acetone, methanol and DMF; very sparingly sol in hexane and petr ether. Substantially insol in water. LD50 in mice (mg/kg): 600 i.p. ; > 2,500 orally (Vezina)

Application (APP):

Tool for immunochemistry.

Therapeutic Codes (THER):

Immunosuppressant; antirestenotic.

Referenced Patent (RPN):

DE2347682; US3929992

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

3.47

11.29

STN INTERNATIONAL LOGOFF AT 22:18:55 ON 26 MAR 2008